Matrix isolation spectroscopy of H_2 in C_{60}

Stephen FitzGerald

Dept. of Physics & Astronomy, Oberlin College, Oberlin OH 44074

Abstract

Solid C_{60} is an ideal host for performing matrix isolation studies on trapped individual molecules. The lattice contains highly uniform, well-separated (10 Å) voids, which are just large enough (4.2Å) to accept a single gas molecule. Given the present interest in hydrogen storage we have used both neutron and infrared spectroscopy to probe the quantum dynamics of H_2 molecules trapped within these voids. Results indicate that even below 10 K the hydrogen rotates almost completely freely while undergoing quantized translational motion back and forth within the cavity. Similarly the vibrational excitation energy is significant red-shifted relative to free hydrogen. Each of these results can then be directly compared to recent theoretical models for the interactions of hydrogen with C_{60}.